

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

1. REPORT DATE (DD-MM-YYYY)

11 April 2003

2. REPORT TYPE

Abstract

3. DATES COVERED (From - To)**4. TITLE AND SUBTITLE**

Polynitrogen Chemistry

5a. CONTRACT NUMBER

F04611-99-C-0025

5b. GRANT NUMBER**5c. PROGRAM ELEMENT NUMBER****6. AUTHOR(S)**

Karl Christie, et al.

5d. PROJECT NUMBER

DARP

5e. TASK NUMBER

A205

5f. WORK UNIT NUMBER**7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**

ERC, Inc.
10 E. Saturn Blvd.
Edwards AFB, CA 93524-7680

**8. PERFORMING ORGANIZATION
REPORT NUMBER****9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)**

Air Force Research Laboratory (AFMC)
AFRL/PRS
5 Pollux Drive
Edwards AFB CA 93524-7048

**10. SPONSOR/MONITOR'S
ACRONYM(S)****11. SPONSOR/MONITOR'S
NUMBER(S)**

AFRL-PR-ED-AB-2003-096

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES**14. ABSTRACT**

20030618 063

15. SUBJECT TERMS**16. SECURITY CLASSIFICATION OF:****a. REPORT**

Unclassified

b. ABSTRACT

Unclassified

c. THIS PAGE

Unclassified

**17. LIMITATION
OF ABSTRACT**

A

**18. NUMBER
OF PAGES****19a. NAME OF RESPONSIBLE
PERSON**

Sheila Benner

**19b. TELEPHONE NUMBER (include
area code)**

(661) 275-5963

FILE

MEMORANDUM FOR PRS (In-House Contractor Publication)

FROM: PROI (STINFO)

21 Apr 2003

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2003-096**
Christe, Karl (ERC) et al., "Polynitrogen Chemistry"

5194

Molecular Dynamics Conference

(Statement A)

17

(San Diego, CA, 18-20 May 2003) (Deadline: 08 Apr 2003)

Polynitrogen Chemistry

Karl Christe, William Wilson, Ashwani Vij, Vandana Vij, Robert Corley, Jerry Boatz, Stefan Schneider, Thorsten Schroer, Ross Wagner, Ralf Haiges, David Dixon, David Feller, Mark Gordon, Heather Netzloff, and Don Jenkins

ERC and Space and Missile Propulsion Division, Air Force Research Laboratory Edwards Air Force Base, CA 93524, Loker Research Institute, University of Southern California, Los Angeles, CA 90089, Pacific Northwest National Laboratory, Richland WA 99352, Department of Chemistry, Iowa State University, Ames, IA 50011, and Department of Chemistry, University of Warwick, Coventry CV4 7AL, UK

karl.christe@edwards.af.mil

Under combined DARPA, AFOSR, NSF, and DOE sponsorship, we have continued our work in polynitrogen chemistry. We have successfully prepared and characterized numerous polyazido compounds, such as $\text{As}(\text{N}_3)_3$, $\text{Sb}(\text{N}_3)_3$, $\text{As}(\text{N}_3)_5$, $\text{Sb}(\text{N}_3)_5$, $\text{As}(\text{N}_3)_6^-$, $\text{Sb}(\text{N}_3)_6^-$, $\text{Te}(\text{N}_3)_4$, $\text{Te}(\text{N}_3)_6^{2-}$, $\text{P}(\text{N}_3)_6^-$, and $\text{B}(\text{N}_3)_4^-$, and have studied the combination of N_5^+ with some of these anions. Most of these compounds are extremely energetic and shock sensitive.

We have studied the reactions of the NF_4^+ and N_2F_3^+ cations with HN_3 in HF solution. The synthesis of the N_7^- anion was also pursued by preparing and characterizing R_3SiNCl_2 and $(\text{R}_3\text{Si})_2\text{NCl}$ compounds. Although their chlorine atoms could not be replaced by azido groups, the reaction of the latter with HF/MF_5 resulted in the isolation of salts of the novel monochloroammonium cation.

Enthalpies of formation were calculated for gas phase N_3 , N_3^- , N_5^+ , and N_5^- from *ab initio* molecular orbital theory. Stability calculations were carried out for solid N_5^+N_3^- and N_5^+N_5^- , using these values and lattice energy estimates.

The possible existence of FN_5 was studied both experimentally by FT-IR spectroscopy of the volatile decomposition products from the thermolysis of $(\text{N}_5^+)_2\text{SnF}_6^{2-}$ and computationally using a RRKM analysis.